

10/542870

=> s l11
SAMPLE SEARCH INITIATED 15:30:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 1 TO 80

L12 1 SEA SSS SAM L11

=> s l11 sss ful
FULL SEARCH INITIATED 15:30:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.01

L13 10 SEA SSS FUL L11

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
166.94 762.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
CA SUBSCRIBER PRICE ENTRY SESSION
0.00 -36.00

FILE 'CAPLUS' ENTERED AT 15:30:57 ON 04 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

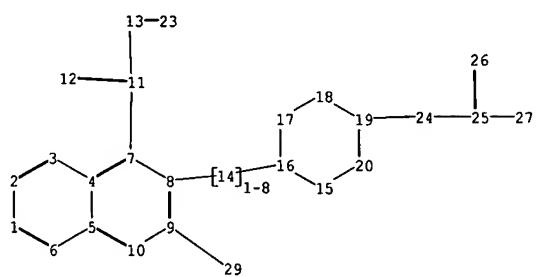
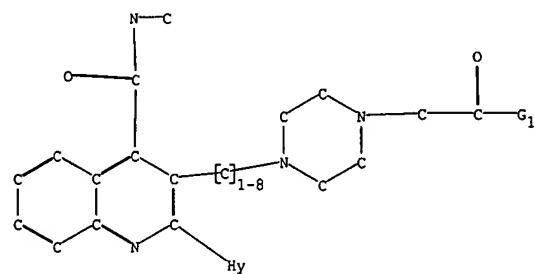
FILE COVERS 1907 - 4 Mar 2006 VOL 144 ISS 11
FILE LAST UPDATED: 3 Mar 2006 (20060303/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l13
L14 1 L13

=> d l14 bib abs hitstr



chain nodes :

11 12 13 14 23 24 25 26 27 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

7-11 8-14 9-29 11-12 11-13 13-23 14-16 19-24 24-25 25-26 25-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18
18-19 19-20

exact/norm bonds :

9-29 11-12 11-13 13-23 14-16 15-16 15-20 16-17 17-18 18-19 19-20 19-24 25-26
25-27

exact bonds :

7-11 8-14 24-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

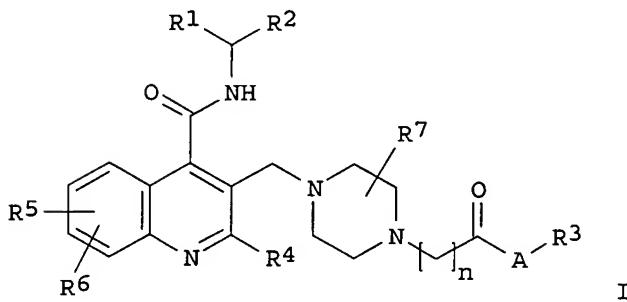
G1:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 29:Atom

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:648345 CAPLUS
 DN 141:190803
 TI Preparation of quinoline derivatives as NK-2 and NK-3 receptor antagonists
 IN Kerns, Jeffrey; Jin, Qi; Wan, Zehong; Nie, Hong; Zhu, Chongjie
 PA Smithkline Beecham Corporation, USA
 SO PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004066950	A2	20040812	WO 2004-US2366	20040129
	WO 2004066950	A3	20041104		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI EP 1601360	A2	20051207	EP 2004-706434	20040129
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRAI	US 2003-443650P	P	20030130		
	WO 2004-US2366	W	20040129		
OS	MARPAT 141:190803				
GI					



AB The title compds. [I; R1 = H, (un)substituted alkyl; R2 = (un)substituted aryl, cycloalkyl, heterocyclyl; R3 = H, (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl; A = NR8, O (R8 = H, (un)substituted alkyl); R4 = (un)substituted heterocyclyl; R5 = H, alkyl, alkenyl, aryl, etc.; or R5 represents a bridging moiety which is arranged to bridge two adjacent ring atoms, wherein the bridging moiety comprises alkylene or dioxyalkylene; R6 = H, halo; R7 = oxo; n = 1-4] which are NK2 and NK3 receptor antagonists and are useful in the treatment of respiratory diseases, were prep'd. E.g., a 4-step synthesis of 3-(4-dimethylcarbamoylmethyl-3-oxopiperazin-1-ylmethyl)-2-(thiophen-2-yl)quinoline-4-carboxylic acid [(S)-1-cyclohexylethyl]amide, was given. The most potent compds. I show IC50 in the range 10-1000 nM against NK-3 receptor binding, and IC50 in the range 1-1000 nM against NK-2 receptor binding. The pharmaceutical compn. comprising the compd. I is claimed.

IT 737804-27-2P 737804-30-7P 737804-36-3P

737804-40-9P 737804-41-0P 737804-42-1P

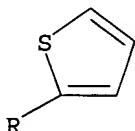
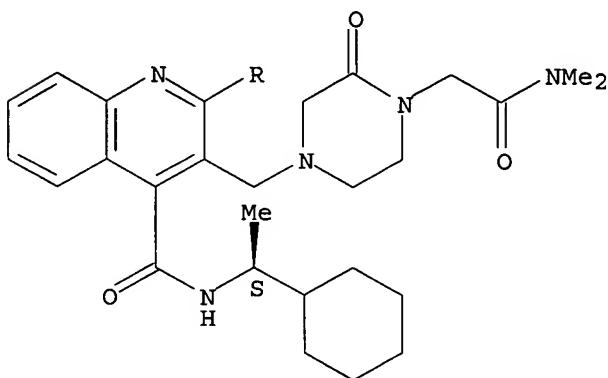
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinoline derivs. as NK-2 and NK-3 receptor antagonists for treating respiratory diseases)

RN 737804-27-2 CAPLUS

CN 4-Quinoliniccarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-(dimethylamino)-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

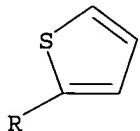
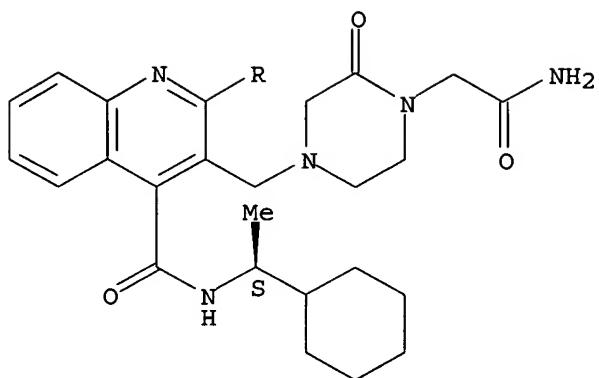
Absolute stereochemistry.



RN 737804-30-7 CAPLUS

CN 4-Quinoliniccarboxamide, 3-[[4-(2-amino-2-oxoethyl)-3-oxo-1-piperazinyl]methyl]-N-[(1S)-1-cyclohexylethyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

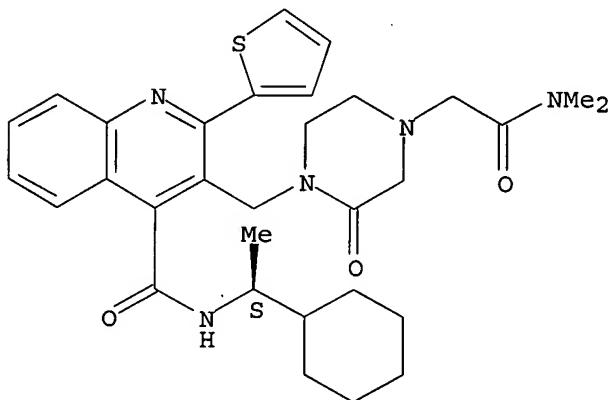
Absolute stereochemistry.



RN 737804-36-3 CAPLUS

CN 4-Quinolinecarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-(dimethylamino)-2-oxoethyl]-2-oxo-1-piperazinyl]methyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

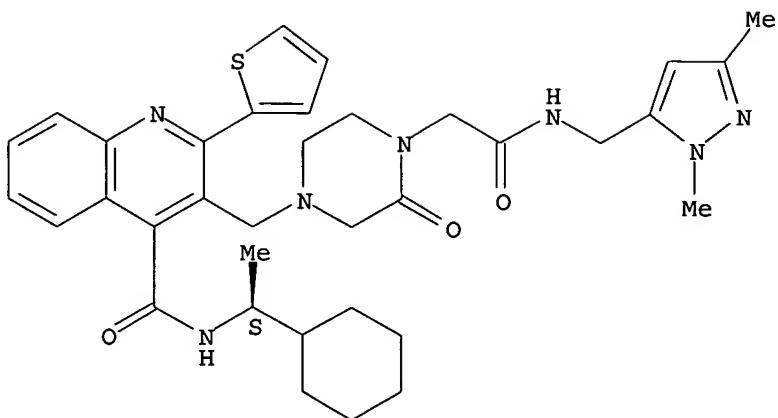
Absolute stereochemistry.



RN 737804-40-9 CAPLUS

CN 4-Quinolinecarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-[(1,3-dimethyl-1H-pyrazol-5-yl)methyl]amino]-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

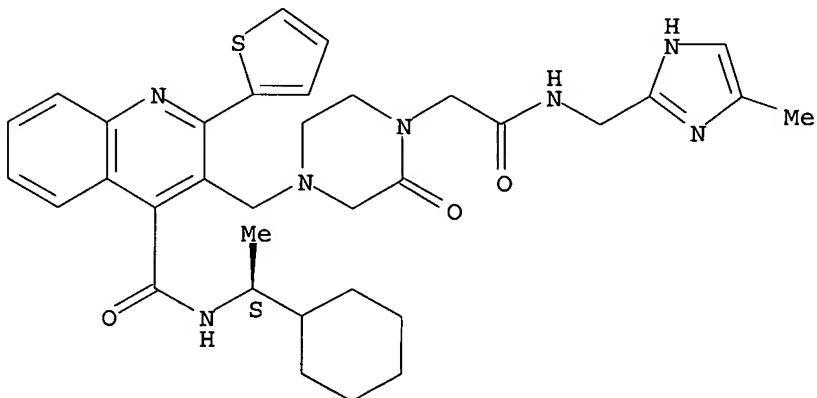
Absolute stereochemistry.



RN 737804-41-0 CAPLUS

CN 4-Quinolinicarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-[[[4-methyl-1H-imidazol-2-yl)methyl]amino]-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)- (9CI) (CA INDEX NAME)

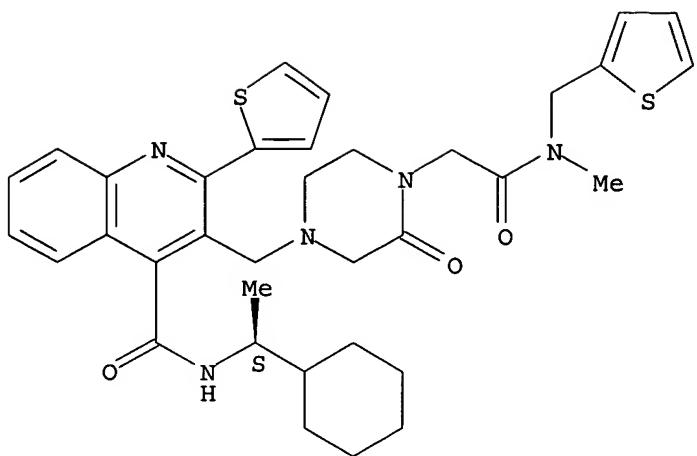
Absolute stereochemistry.



RN 737804-42-1 CAPLUS

CN 4-Quinolinicarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-[methyl(2-thienylmethyl)amino]-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



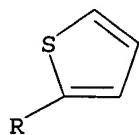
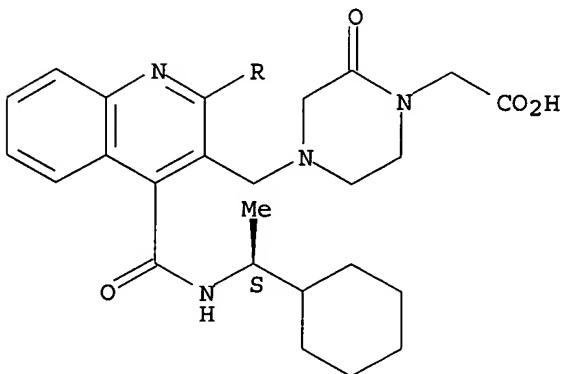
IT 737804-43-2P 737804-46-5P 737804-47-6P
737804-48-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of quinoline derivs. as NK-2 and NK-3 receptor antagonists for treating respiratory diseases)

RN 737804-43-2 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-(2-thienyl)-3-quinolinyl]methyl]-2-oxo- (9CI) (CA INDEX NAME)

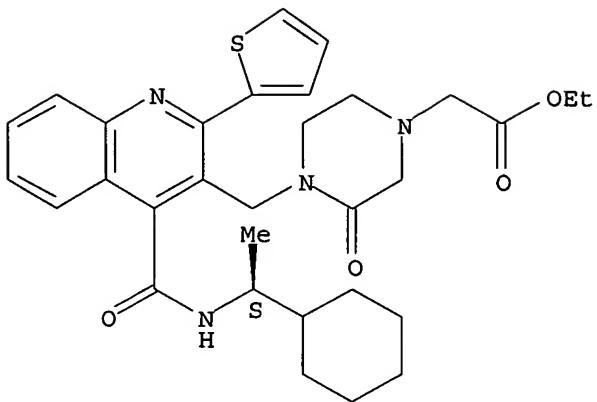
Absolute stereochemistry.



RN 737804-46-5 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-(2-thienyl)-3-quinolinyl]methyl]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)

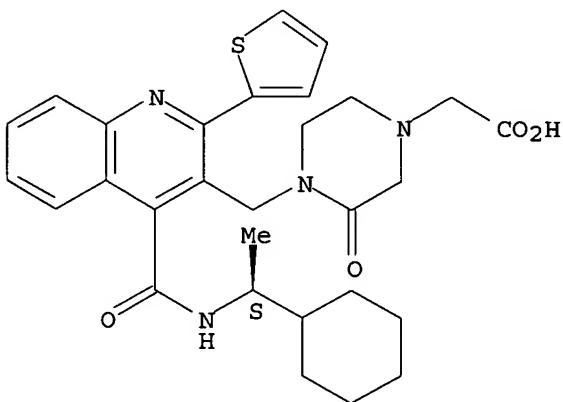
Absolute stereochemistry.



RN 737804-47-6 CAPLUS

CN 1-Piperazineacetic acid, 4-[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-(2-thienyl)-3-oxo- (9CI) (CA INDEX NAME)

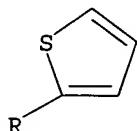
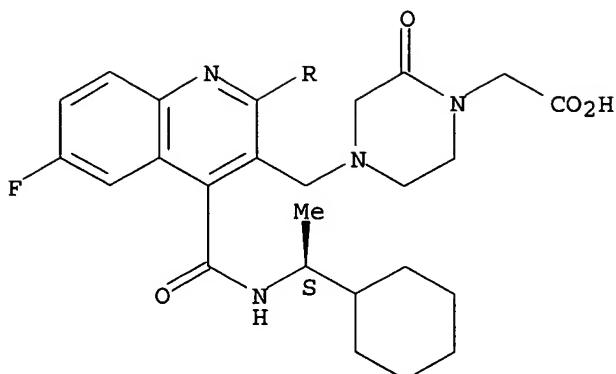
Absolute stereochemistry.



RN 737804-48-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-6-fluoro-2-(2-thienyl)-3-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> file caold			
COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
FULL ESTIMATED COST	ENTRY	SESSION	
	5.57	768.06	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL	
CA SUBSCRIBER PRICE	ENTRY	SESSION	
	-0.75	-36.75	

FILE 'CAOLD' ENTERED AT 15:31:14 ON 04 MAR 2006
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

```
=> s 113
L15          0 L13

=> log h
```

10/542870

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.44	768.50
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-36.75

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 15:31:21 ON 04 MAR 2006

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1594	((544/121) or (544/357)).CCLS.	US-PGPUB; USPAT	OR	OFF	2006/03/04 21:12
L2	465	NK-2 or NK-3	US-PGPUB; USPAT	OR	OFF	2006/03/04 21:12
L3	8	I1 and I2	US-PGPUB; USPAT	OR	OFF	2006/03/04 21:12